# Consequential cradle-to-gate carbon footprint of water treatment chemicals using simple and complex marginal technologies for electricity supply

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## Abstract

*Purpose* Chemicals produced via chlor-alkali electrolysis are widely used throughout the water industry worldwide, with treatment chemicals often the second largest source of environmental impacts from potable water production after electricity use. Population-driven increases in the future demand for potable water will require concomitant increases in the production of water treatment chemicals, with the associated environmental impacts of chemicals production primarily arising from the additional demand for electricity. Due to the dominance of electricity in the environmental performance of chlor-alkali chemicals, assessment of the future environmental impacts of potable water production is largely dependent on proper identification of the marginal source of electricity. In this paper, we present a consequential cradle-to-gate carbon footprint (cCF) for the most widely used chlor-alkali-produced disinfectant (sodium hypochlorite (13 % *w/w*)) and coagulant (ferric chloride (42 % *w/w*)) in Australia, with special emphasis placed upon the identification of future marginal electricity supply and the substitution of hydrogen gas and sodium hydroxide during production. While this analysis is presented in an Australian context, commonalities in potable water and chlor-alkali chemical production processes internationally give the findings a broader relevance.
*Methods* Consequential models for sodium hypochlorite (13 % *w/w*) and ferric chloride (42 % *w/w*) production were developed, and the identification of the marginal source of electricity was modelled using a "simple marginal technology" approach via operationalisation of the Weidema framework and a "complex marginal technology" using a partial equilibrium model. For the simple marginal technology, the levelised cost of electricity was used to select the most competitive energy generation technologies and those most relevant for the Australian market. For the complex marginal technology, the energy sector model was used to simulate the most likely electricity supply mix. Details of the different paths taken in the substitution of hydrogen gas and sodium hydroxide are also presented. To allow for proper incorporation of uncertainties arising from these key factors in the cCF, several scenarios were developed covering fuel and carbon prices for identifying the marginal supply mix of electricity, as well as the likely production routes for sodium carbonate in the context of sodium hydroxide substitution.
*Results and discussion* cCF results of sodium hypochlorite (13 % *w/w*) and ferric chloride (42 % *w/w*) are presented using simple and complex marginal technologies, and the implications of choosing one marginal technology over the other in the context of water treatment chemicals are presented. For the simple marginal technology approach, the global warming potential (GWP) per megagram of chemical varied from 68 to 429 kg $CO_2$-eq for sodium hypochlorite (13 % *w/w*) and

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59–1,020 kg $CO_2$-eq for ferric chloride (42 % *w/w*). For the complex marginal technology approach, the GWP per megagram of chemical varied from 266 to 332 kg $CO_2$-eq for sodium hypochlorite (13 % *w/w*) and 214–629 kg $CO_2$-eq for ferric chloride (42 % *w/w*). Insights are given in relation to the impact of the price of fossil fuels, the carbon price, and the different substitution routes.

*Conclusions* The use of a partial equilibrium model (PEM) has enabled a better understanding of the variability of the results in this study. For example, the use of PEM for the identification of the complex marginal source of electricity shows that, for the case of Australia, any benefit from a carbon price is lost with high prices of natural gas due to the incentive to use cheaper fuels such as black and brown coal. Likewise, the use of explorative scenarios was decisive to manage the inherent uncertainty of the parameters included in the model. In relation to substitution, the case of ferric chloride (42 % *w/w*) indicated that using only one substitution route was not enough to fully understand the potential continuum of cCF results. The simple marginal approach, where an exclusive marginal source of electricity or substitution route is considered, presents significant risks for the modelling accuracy of the cCF as shown here for sodium hypochlorite (13 % *w/w*) and ferric chloride (42 % *w/w*), therefore, it is not recommended.

**Keywords** Chlor-alkali chemicals · Coagulation and disinfection · Consequential carbon footprint · Potable water treatment

# 1 Introduction

One of the most important industrial processes associated with the supply of potable water is the manufacturing of chlor-alkali chemicals. The chlor-alkali electrolysis process is the exclusive route for the production of chlorine gas needed in the manufacture of sodium hypochlorite (13 % *w/w*) and ferric chloride (42 % *w/w*) which are widely used during chemical disinfection and coagulation of water. The future demand of water treatment chemicals is expected to grow as a consequence of the projected increases in potable water demand linked to population growth. In the case of Australia, total future urban water consumption in major cities is expected to grow from 1,505 GL in 2009 to between 2,467 and 3,117 GL per year by 2030, depending on population growth estimates (WSAA 2010). This represents an estimated additional demand of some 25,730 Mg of sodium hypochlorite (13 % *w/w*) and 18,800 Mg of ferric chloride (42 % *w/w*) by 2030 for potable water disinfection in the eastern seaboard of Australia alone.

Previous life cycle assessments (LCAs) have looked at the environmental impacts of the chlor-alkali process using an attributional approach in areas related to solid waste (Muñoz and Navia 2011), electrolysis technology (Jung et al. 2013)

and allocation (Alvarez-Gaitan et al. 2014). However, these studies have applied an "accounting" perspective which is limited in the evaluation of environmental impacts associated with changes in the production of these chemicals as a result of changes in the demand (e.g. potable water in the long-term). Water utilities wishing to operate under ecologically sustainable development principles and wanting to strategically evaluate the greenhouse gas (GHG) emissions embedded in the consumption of chlor-alkali chemicals during future potable water production need to include market information in LCAs conducted for such strategy and planning activities, in other words, switching from an 'attributional' to a 'consequential' approach (ILCD 2010).

Indirect effects have to date been included in CLCIs using different techniques. Originally, the Weidema step-wise procedure (Weidema 2003) was the principal methodological framework in consequential studies. Later, other approaches such as computable general equilibrium and partial equilibrium modelling (PEM) were used to provide robustness to the modelling phase (Zamagni et al. 2012). More recently, some studies have compared the results obtained using these tools under different assumptions (Vázquez-Rowe et al. 2013) showing the advantages and drawbacks of each or evaluating the different approaches available for CLCI modelling (Marvuglia et al. 2013). For water treatment chemicals, the use of electricity during chlor-alkali production represents not only a fundamental resource input and cost to production facilities but is also the main source of environmental impacts; this is especially true for countries like Australia, where electricity is generated primarily from coal (Alvarez-Gaitan et al. 2013a). As such, the scale of the environmental impacts from chlor-alkali chemicals production in a CLCI framework depends to a large extent on proper identification of the marginal source of electricity.

Previous CLCIs have identified the marginal source of electricity simply on the basis of what is the most cost-competitive technology—generally natural gas (Schmidt et al. 2007; Thomassen et al. 2008) or coal (Gaudreault et al. 2010; Skals et al. 2008). However, in the context of complex interactions of various generation technologies in day-to-day grid operations, Mathiesen et al. (2009) suggests the use of simple and complex marginal technologies, ideally within an energy systems scenario analysis framework; this breadth of analysis requires the use of economic modelling tools such as PEMs.

Another important consideration in CLCIs is the treatment of multifunctional processes, such as in the case of chlorine gas production where sodium hydroxide and hydrogen gas need to be substituted. This represents an important source of uncertainty for such analyses due to the incorporation of other supply chains and the use of market mechanisms to identify the most likely substituted processes. While literature examples of multifunctional output substitution in CLCIs are particularly abundant for agricultural products such as biofuels,

they are comparatively scarce for water treatment chemicals (Zamagni et al. 2012), limiting the development and acceptance of cCF in the water industry.

To address the above knowledge gaps, we present a consequential cradle-to-gate carbon footprint of increased production of sodium hypochlorite (13 % w/w) and ferric chloride (42 % w/w) associated with elevated future demand for potable water in Australia in the year 2030. Given the dominance of electricity use in the environmental impacts of chlor-alkali production, particular emphasis is given here to how the marginal source of electricity is identified.

# 2 Methods

## 2.1 Goal and scope definition

In this article, we aim to provide an answer to the following question: What would be the environmental impacts associated with an increase in the production of sodium hypochlorite (13 % w/w) and ferric chloride (42 % w/w) as a result of a higher demand of potable water on the Australian east coast?. The study is limited to GWP to highlight the role played by electricity in the chlor-alkali process in general and the use of coal-fired electricity in Australia in particular. The functional unit of this cCF is an additional production of 1 Mg of sodium hypochlorite (13 % w/w) and 1 Mg of ferric chloride (42 % w/w) in Australia linked to increased potable water demand in 2030. Two different approaches for identifying the future marginal source of electricity are used: Weidema's five-step approach, named here as "identification of simple marginal technologies", and PEM, named here as "identification of complex marginal technologies". Specific details are provided on the single versus multiple substitution routes in dealing with the multifunctionality of the chlor-alkali process. Two chlor-alkali-produced chemicals previously identified as widely used in Australia for potable water disinfection and coagulation (i.e. sodium hypochlorite (13 % w/w) and ferric chloride (42 % w/w), respectively (Alvarez-Gaitan et al. 2011)), are used as case studies.

## 2.2 System boundaries

Figures 1 and 2 present the system boundaries of the case study chemicals sodium hypochlorite (13 % w/w) and ferric chloride (42 % w/w), respectively. The systems included in the assessment are shown, along with the points of displacement.

## 2.3 Identification of simple marginal technologies—the five-step Weidema approach

The five-step approach to consequential analysis outlined by Weidema (2003) has been commonly used

in CLCIs for agricultural products (Dalgaard et al. 2008) and biofuels (Reinhard and Zah 2009). Each of these five steps is presented below, with a detailed discussion of the rationale behind each step.

### 2.3.1 What time horizon applies to the study?

The focus is specifically on the long-term consequences, because any increase in demand for these chemicals in the short term will affect only existing production capacity whereas, in the longer term, it will require the installation of new capacity which reflects the most common and persistent effect (Weidema et al. 2009). Consequently, as we are evaluating the additional demand for electricity associated with an increase in the production of chlor-alkali chemicals linked to additional demand of potable water in 2030, the emphasis is on the long-term marginal supply of electricity, given its overbearing contribution toward the environmental impacts of chlor-alkali production (Alvarez-Gaitan et al. 2013a). The contribution of other inputs, such as salt, water and ancillary materials, are considered of minor importance, and so, the marginal suppliers for these materials are considered to remain unchanged during the modelled timeframe.

### 2.3.2 Does the change only affect specific processes or a market?

The studied change is considered small as the additional demand is not expected to have an impact in the overall market trend. New capacity for chlorine gas production is dominated by the installation of membrane cell technology, which is the technology currently used in Australian chlor-alkali facilities. Figure 3 shows the current and recent historical market trends for mercury, diaphragm and membrane cell technologies in Europe. Together, these data strongly suggest that membrane cell technology is likely to dominate during the coming decade at least. For the purposes of our analysis, we consider that membrane cells are also the technology of choice in new installations out to 2030. The additional demand for sodium hypochlorite (13 % w/w) and ferric chloride (42 % w/w) will increase the demand for chlorine gas in Australia, which will be satisfied by local production due to the high cost of shipping chlorine gas by sea (EIPPCB 2013). This market assumption is supported by data of the United Nations COMTRADE database, wherein Australia has imported no more than 660 Mg of chlorine per year during the last 20 years (United Nations 2013).

### 2.3.3 What is the trend in the volume of the affected market?

At the foreground level, the demand for chlorine is expected to increase as a result of additional demand for chlor-alkali
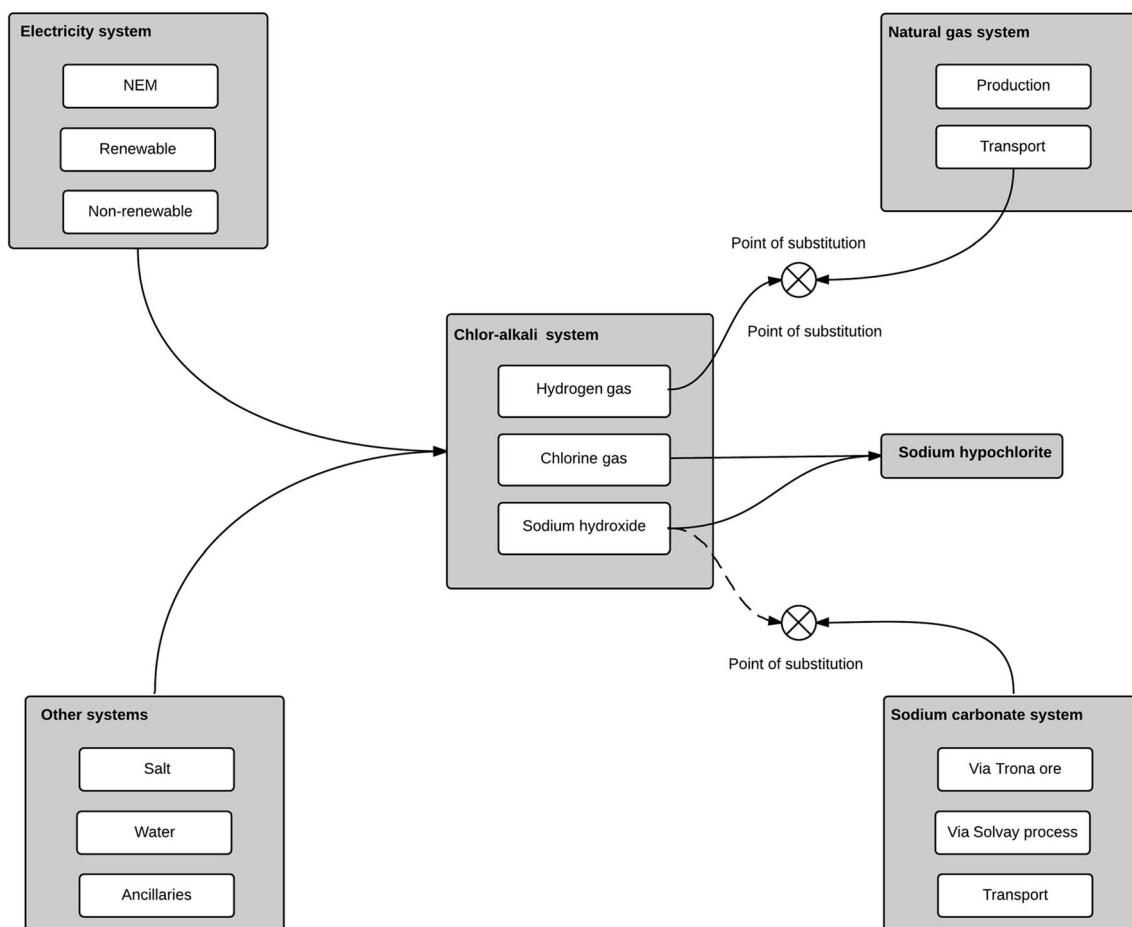
**Fig. 1** System boundaries associated with the production of sodium hypochlorite (13 % *w/w*) including the points of substitution

chemicals. At the background level, however, it is necessary to understand that the Australian National Electricity Market (NEM) comprises an electricity network covering around 5,000 km of the Eastern seaboard from South Australia to Queensland and includes Tasmania through the BassLink interconnector. Currently, 75 % of national electricity demand is satisfied by coal-fired power generators (AER 2013). In the NEM, electricity supply and demand are matched in real-time through a central clearing mechanism following the merit order effect. As shown in Fig. 4, the total 2013 demand forecast differed considerably from that of 2012 due to the continuation of a declining consumption trend established in 2007–2008, seen as a result of reduced industrial electricity consumption (linked to the high Australian dollar) and reduced residential consumption due to substantial increases in retail electricity prices combined with the broad uptake of domestic photovoltaic systems. However, the demand for electricity is expected to continue to grow in the long-term under all scenarios according to the most recent National Energy Forecasting Report (AEMO 2013). Here, we assume that the future demand for electricity is slowly growing at best or at worst steady.

*2.3.4 Is there potential to provide an increase or reduction in production capacity?*

At the foreground level, the production of chlorine gas using the affected technology (membrane cells) is unconstrained and can only be provided by local manufacturing. Therefore, the installation of new chlor-alkali capacity will require additional supply of electricity from the NEM as described in step 3 where the respective market trend was identified. In order to identify those technologies likely to be able to satisfy future increases in electricity demand, we need to first isolate and exclude those with constrained production capacity within the Australian context (Table 1).

*2.3.5 Is the technology the most/least preferred?*

The Australian Energy Technology Assessment (AETA) reports (BREE 2012; BREE 2013) were used to identify the competitiveness of different electricity technologies with and without pricing carbon dioxide emissions. These reports present a detailed picture of 40 electricity-generation technologies hierarchised using the levelised cost of energy (LCOE) which
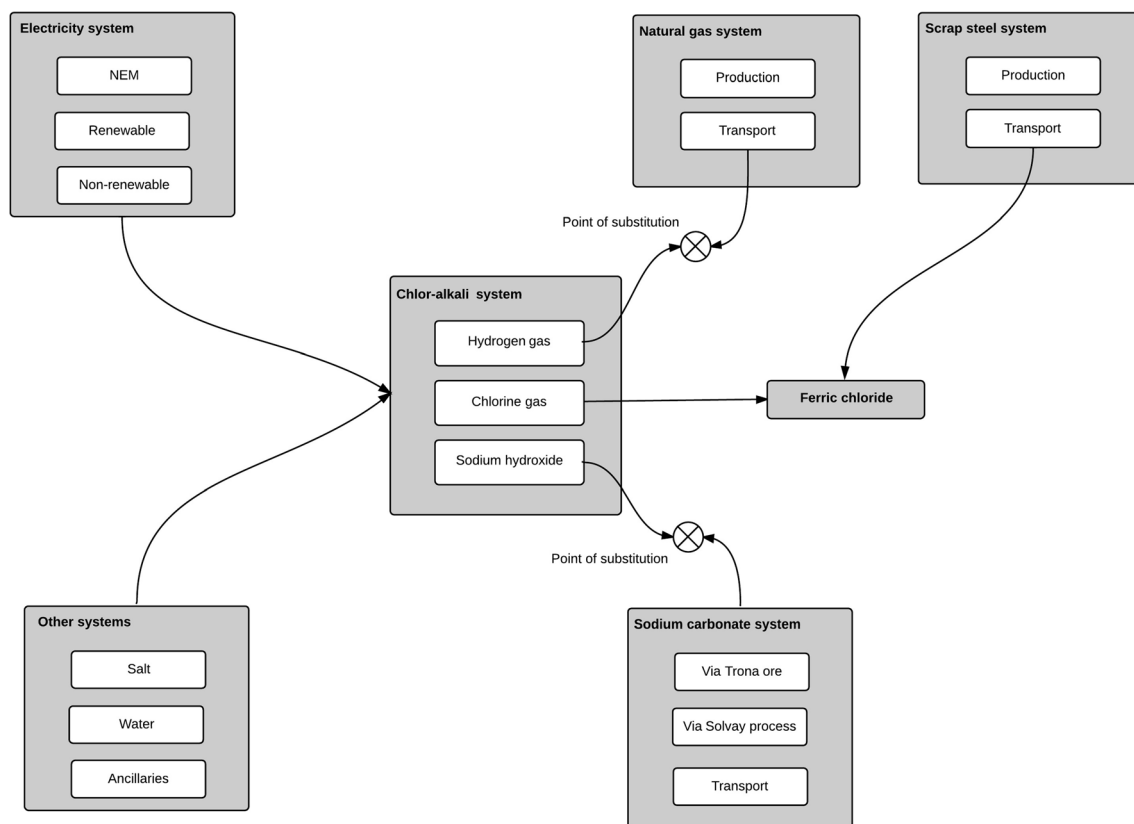
**Fig. 2** System boundaries associated with the production of ferric chloride (42 % *w/w*) including the points of substitution

includes capital costs (local and international components), and operation and maintenance costs (fixed and variable, carbon price, fuel costs, carbon sequestration and storage and owner's costs). All the technologies were considered to be used at utility-scale only (typical new entrant size >100 MW). Items not included were decommissioning and network/transmission costs. Table 2 presents the 2030 LCOE in Australian dollar per megawatt-hour (A\$/MWh) for the different technologies with and without a carbon price. Price on carbon dioxide emissions estimated to be around \$ 45/Mg
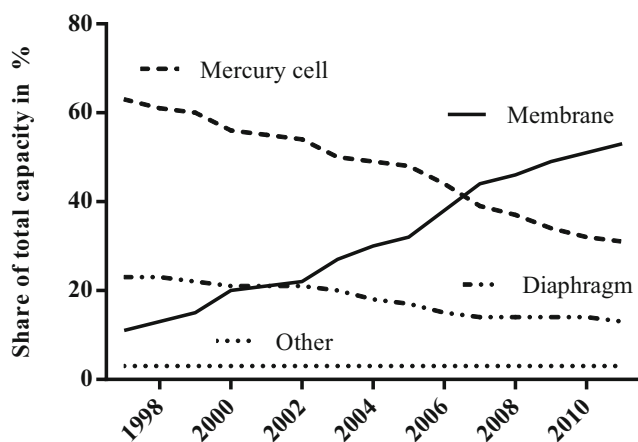
$CO_2$-eq following the strong growth low pollution (SGLP) scenario (Australian Government 2011).

Both AETA reports estimate that by 2030, wind (onshore) and solar PV (non-tracking) will have the lowest LCOE of all the renewable technologies assessed. Of all the fossil-fuelled technologies, supercritical pulverised black coal appears to be



**Fig. 3** Relative European chlorine production capacity of the various chlor-alkali technologies during the period 1997–2011 (EIPPCB 2013)
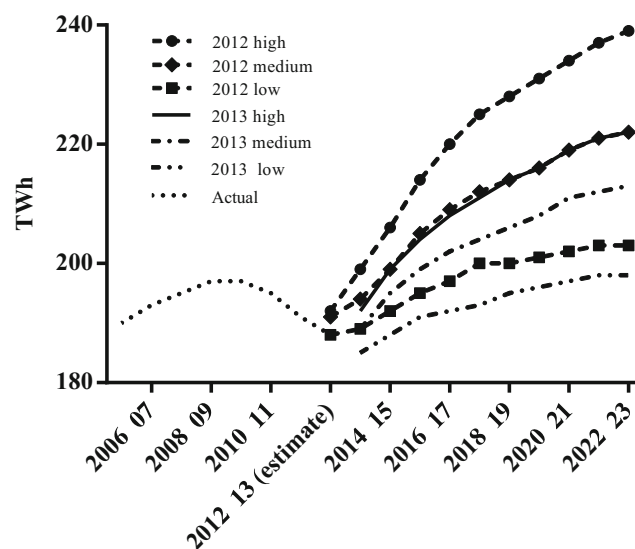


**Fig. 4** Historical (2005–2012) and future (2013–2022) demand of electricity in Australia estimated in 2012 and 2013 under low, medium and high demand scenarios (AEMO 2013)

**Table 1** Electricity technologies with production capacity constraints in Australia

| Technology | Why is it constrained? | Source |
|---|---|---|
| Hydroelectricity | Existing hydroelectric facilities are installed at the most suitable locations for large scale generation. Low and variable rainfall is expected in the future in many regions due to projected climatic change. | (Geoscience Australia 2010) |
| Nuclear electricity | Australia currently has no nuclear power reactors and no plans to build any. The Australian Radiation Protection and Nuclear Safety Act of 1998 prohibits the construction of new nuclear power plants in the country. | (Owen 2011) |
| Biomass-based electricity | Under the most optimistic "high technology change" scenario, only 40 % of the total electricity demand in 2010 could have been satisfied using a combination of different biomass resources. Municipal solid waste incinerators are not accepted by Australian cities. | (Crawford et al. 2012) |

the most competitive followed by pulverised brown coal and combined cycle gas turbine. While health costs and potential investments risks associated with "unburnable carbon" have not been included in the analysis, it is expected that these factors will most likely only serve to make renewables even more attractive than fossil-fuelled technologies in the future. As others have indicated, however, all of the potential technologies supplying electricity to the grid are part of a wider system (Lund et al. 2010), and as such, the long-term marginal electricity supply is likely to comprise a mix of generation technologies. Accordingly, and echoing the earlier sentiments of Mathiesen et al. (2009), we have estimated the complex marginal technology in 2030; this is particularly challenging due to, among other things, the incorporation of new-generation technologies in future supply.

### 2.4 Identification of complex marginal technologies—partial equilibrium modelling approach

A suitable tool for the identification of this "complex marginal technology" in the Australian economy is the Energy Sector Model developed by the CSIRO which is a PEM of the electricity generation and transport sectors solved as a linear program in order to simulate real-life investment decisions (Graham et al. 2013). The estimation of the complex marginal technology requires an iterative process to achieve the lowest

**Table 2** LCOE (Autralian dollar per megawatt-hour) for different technologies in 2030 with and without carbon price

| Technology | With carbon price | Without carbon price |
|---|---|---|
| Solar/coal hybrid | 125–180 | 60–110 |
| Supercritical pulverised black coal | 125–200 | 60–110 |
| Wind onshore | 60–125 | 60–125 |
| Direct injection coal engine | 125–180 | 75–120 |
| Supercritical pulverised brown coal | 150–240 | 70–125 |
| Combined cycle gas turbine | 90–165 | 75–130 |
| Solar photovoltaic–non-tracking | 45–170 | 45–170 |

cost possible for the infrastructure in place, while also satisfying the reliability standard for the system. The Energy Sector Model PEM uses an interface called 'efuture' (CSIRO 2012) which enables users to choose between different levels of electricity demand, fuel prices and cost of technologies. It also includes peak or storage backup capability, as well as a nuclear power option. While carbon price simulation is not an option in the efuture tool, the CSIRO kindly supplied on request the output of the Energy Sector Model with and without this parameter. Following on from what was discussed in Section 2.3, the scenarios and levels of parameters used for identification of the "complex marginal technology" here are shown in Table 3.

The efuture tool has thousands of parameters, many of them relying on qualified assumptions. For example, the model uses mid-range estimates regarding the efficiency of power stations and does not have uncertainty bounds which could make possible the comparison of mid-range against low- and high-range estimate outcomes. Therefore, a comprehensive evaluation of the uncertainty associated with each parameter and its potential combinations with other parameters in the model, while feasible, is not included here. However, the magnitude of the uncertainty associated with the outputs of the model is carried out using explorative scenarios (e.g. Höjer et al. (2008)). For the electricity supply, the price of fossil fuel and the inclusion/exclusion of a carbon price are seen as the most relevant parameters for our analysis. The output from the PEM is shown in Table 4.

### 2.5 Substitution of sodium hydroxide and hydrogen gas

In the chlor-alkali process, chlorine gas, sodium hydroxide and hydrogen gas are produced simultaneously. The determining product from the chlor-alkali facility is chlorine gas and any additional demand of chlor-alkali chemicals such as sodium hypochlorite (13 % $w/w$) or ferric chloride (42 % $w/w$) will increase the production of the co-products hydrogen gas and sodium hydroxide. Sodium carbonate is the most likely substitute of sodium hydroxide as a neutralising agent (Alvarez-Gaitan et al. 2014). Australian production of sodium

**Table 3** Scenarios considered in the identification of the complex marginal electricity technology using the efuture tool

| Scenario | Fuel price | Carbon price | Electricity demand | Technology cost | Nuclear | Peak back-up |
|---|---|---|---|---|---|---|
| 1 | Low | Yes | Low | Medium | No | Yes |
| 2 | Low | No | Low | Medium | No | Yes |
| 3 | High | Yes | Low | Medium | No | Yes |
| 4 | High | No | Low | Medium | No | Yes |

carbonate is expected to cease from 2013 (The Australian 2013); therefore, sodium carbonate to be substituted in the future will most likely be sourced internationally.

There are two different production routes for sodium carbonate: via the Solvay process and from Trona ore mining (USGS 2011). Nevertheless, the UN COMTRADE database (United Nations 2013) shows that the majority of the sodium carbonate imported into Australia comes from the United States, where Trona ore dominates, indicating that this may be the most competitive supplier. Accordingly, we have included this production route for the Weidema approach. For the complex marginal technology scenarios, we are also including the Solvay process in our simulation when substitution is applied, as this is the most popular route for the production of sodium carbonate in China which is the second most popular origin of Australian sodium carbonate.

While Solvay process data are included in the GaBi 6 database (PE International 2013), inventory data regarding the production of sodium carbonate via Trona ore was taken from a previous study on the production of plastic resins in the United States as part of the US life cycle inventory database (Franklin Associates 2011). Although hydrogen is commonly

produced through steam reforming, the amount being produced in the chlor-alkali facility in this study is insufficient to be commercially viable for use in downstream processes (Alvarez-Gaitan et al. 2014). For this reason, hydrogen is burned along with natural gas in some chlor-alkali facilities to evaporate water and increase the concentration of sodium hydroxide coming from the electrolyser from 32 % w/w to around 50 % w/w. As a result, the most likely process to be substituted is the production of natural gas which is commonly used for combustion in boilers (Alvarez-Gaitan et al. 2014).

In the case of ferric chloride (42 % w/w), a source of iron is required. Usually, this comes from a combination of spent pickle liquor and steel scrap, whereby the latter supplies 93 % of the iron input. Scrap behaves as a global commodity, and the latest figures from COMTRADE show that, in 2011, Australia exported 1.7 million Mg of ferrous scrap while importing 2,893 Mg (United Nations 2013). These figures indicate that ferrous scrap is primarily sourced locally at competitive prices. The scrap market is extremely important for the production of steel via electric arc furnace (EAF) which can use up to 100 % scrap in the production of steel; for comparison, basic oxygen furnaces can use up to 30 % scrap

**Table 4** Estimated contributions in absolute (TWh) and relative (%) figures per technology to the complex marginal technology in 2030 under different fuel and carbon price scenarios

| Technology[a] | Scenario | | | |
|---|---|---|---|---|
| | 1 | 2 | 3 | 4 |
| Brown coal (BrC) | 32.3 (13.2 %) | 32.3 (13.2 %) | 32.3 (13.2 %) | 32.3 (13.2 %) |
| Direct injection coal engine (DICE) | 4.91 (2.01 %) | 11.7 (4.76 %) | 12.8 (5.2 %) | 10.9 (4.4 %) |
| Black coal (BC) | 88.3 (35.9 %) | 101 (41.1 %) | 92.5 (37.7 %) | 109 (44.3 %) |
| Combined cycle gas turbine (CCGT) | 20.6 (8.37 %) | 4.28 (1.74 %) | 2.06 (0.84 %) | 0.98 (0.40 %) |
| Combined cycle gas turbine with carbon capture and storage | 0 | 0 | 0 | 0 |
| Open cycle gas turbine (OCGT) | 8.51 (3.47 %) | 8.22 (3.35 %) | 8.57 (3.49 %) | 7.47 (3.04 %) |
| Biomass (B) | 7.44 (3.03 %) | 5.95 (2.42 %) | 1.49 (1.49 %) | 1.49 (0.61 %) |
| Hydroelectricity (H) | 13.1 (5.34 %) | 13.1 (5.34 %) | 13.1 (5.34 %) | 13.1 (5.33 %) |
| Wind turbines onshore (W) | 41.5 (16.9 %) | 43.1 (17.5 %) | 51.0 (20.7 %) | 46.3 (18.8 %) |
| Geothermal | 0 | 0 | 0 | 0 |
| Solar thermal with storage (ST) | 1.21 (0.49 %) | 1.09 (0.44 %) | 2.26 (0.92 %) | 2.1 (0.85 %) |
| Large photovoltaic | 0 | 0 | 0.28 (0.11 %) | 0.28 (0.11 %) |
| Rooftop solar photovoltaic (PV) | 19.5 (7.94 %) | 15.3 (5.21 %) | 20.3 (8.25 %) | 14.6 (5.96 %) |
| Other distributed generation (DG) | 8.11 (3.30 %) | 9.76 (3.97 %) | 8.86 (3.61 %) | 7.41 (3.02 %) |

[a] Totals may differ due to rounding

in their production. In Australia, most of the capacity is associated with the basic oxygen furnace route (≈80 %) while the rest is EAF. While there are three sources of steel scrap (i.e. home, new and old scrap, representing 20–30, 15–25 and 40–55 % of the market, respectively) (Yellishetty et al. 2011), only high-quality steel scrap is potentially suitable for the production of ferric chloride (42 % *w/w*) due to the regulation of impurities in water treatment chemicals (NHMRC 2011). As such, the production of ferric chloride (42 % *w/w*) is a price taker rather than a price maker for high-quality steel scrap which is a valuable material for the production of steel via EAF worldwide. The most likely marginal supply of iron in the future will be high-quality postconsumer steel scrap metal, and very limited substitution opportunities exist due to the limited amount of iron in spent pickle liquor and the potential impurities arising from lower grades of steel scrap.

## 3 Results and discussion

Tables 5 and 6 present the cCF results of sodium hypochlorite (13 % *w/w*) and ferric chloride (42 % *w/w*) production calculated according to the two approaches described in Section 2. We have arranged our discussion regarding the benefits and drawbacks of using simple and complex marginal approaches in consequential studies according to the three key factors most relevant to our analysis: carbon price, fuel price and substitution.

### 3.1 Carbon price

When the single marginal technology approach is used, selection of the future marginal technology under a carbon price scenario appears relatively straightforward as the gap between renewables and non-renewables is significant. In contrast, without a carbon price, this choice becomes much more difficult, as the gap in competitiveness between renewable and non-renewable technologies is compressed as shown in Table 2. Without a carbon price, the competitiveness of fossil fuels improves dramatically such that they become similarly competitive to renewables on a LCOE basis. While a 100 % renewable electricity supply is feasible for Australia (Elliston et al. 2012; Elliston et al. 2013), it is perhaps unlikely within the forecast 2030 time horizon and, hence, is beyond the scope of this paper to consider it in any detail.

As can be appreciated in the data of Table 5, the uncertainty in the identification of future marginal electricity supply is crucial in the final results of the chemicals included in this analysis. As expected, the results for sodium hypochlorite (13 % *w/w*) and ferric chloride (42 % *w/w*) production when electricity is sourced from photovoltaics and onshore wind

generation show a considerably lower GWP than when sourced from combined cycle gas turbine, black or brown coal. More importantly, however, the risks of incorrectly choosing one technology over the other as part of the simple marginal technology approach are significant, as is the potential for erroneous outputs from such an analysis. For example, choosing supercritical pulverised black coal (in the absence of a price in carbon dioxide emissions) yields 368 kg $CO_2$-eq per Mg for sodium hypochlorite (13 % *w/w*) and 850 kg $CO_2$-eq per Mg for ferric chloride (42 % *w/w*), respectively. In contrast, if the simple marginal technology chosen is onshore wind, the results are 69 kg $CO_2$-eq per Mg for sodium hypochlorite (13 % *w/w*) and 64 kg $CO_2$-eq per Mg for ferric chloride (42 % *w/w*). Table 6 results show a slightly lower GWP for both chemicals when a carbon price is included in the low fuel price scenario; however, this concession effectively disappears for both chemicals when high fuel prices are used and sodium hydroxide substitute sodium carbonate production via Trona ore. The effects of fuel prices and substitution are further discussed below.

### 3.2 Fuel prices

When the complex marginal technology approach is used, there is an increase in GHG emissions intensity per unit of chemical produced when moving from low to high fuel price scenarios under either sodium carbonate production route for both modelled water treatment chemicals. While this seems counterintuitive, the reason behind this is the potential reversion to coal-fired generation where natural gas prices are too high. As shown in Fig. 5, the anticipated future price of coal (Fig. 5a) and natural gas (Fig. 5b) is expected to follow opposing trajectories out to 2030, with coal prices expected to be lower in the long term while natural gas prices will increase. Higher prices of natural gas magnify the price gap between this fuel and coal, such that power generators are more likely to purchase coal which is a cheap fuel rather than buying a cleaner but comparatively expensive fuel such as natural gas. Due to the dynamics of the market, when the gap between the price of gas and coal is reasonable, as in the low fuel price scenario, relatively more gas-fired electricity is expected in the mix, while the opposite will occur when the price gap widens as in the high fuel price scenario. While this effect is included in the LCOE range for each technology, when the simple marginal technology approach is used for estimating the future environmental impacts of an energy-intensive production process like chlor-alkali chemicals production, the uncertainty and potential for erroneous results from using only one technology and/or not considering probable changes in the future price of fuels, is significant. As demonstrated here, using the complex marginal approach is important to comprehensively estimate long-term changes in cCFs.

**Table 5** cCF results (GWP) in kilograms CO$_2$-eq per megagram of produced sodium hypochlorite (13 % $w/w$) and ferric chloride (42 % $w/w$) using the simple marginal technology approach for electricity supply identification and sodium hydroxide substituting sodium carbonate via Trona ore processing

| Marginal technology | Substitution via | Sodium hypochlorite (13 % $w/w$) | Ferric chloride (42 % $w/w$) |
|---|---|---|---|
| Photovoltaic | Trona ore | 68 | 59 |
| Wind | Trone ore | 69 | 64 |
| Combined cycle gas turbine | Trona ore | 253 | 550 |
| Black coal | Trona ore | 368 | 850 |
| Brown coal | Trona ore | 429 | 1,020 |

### 3.3 Substitution

While it is common in CLCIs to use marginal suppliers based on their competitiveness for substitution purposes, the variability in GWP results here between the two approaches (Tables 5 and 6) highlights the need for scenario modelling as identified previously by Zamagni et al. (2012). Using sodium carbonate produced via Trona ore as the alkali to be substituted by sodium hydroxide in the single marginal technology approach neglects the potential effects of using a different production path for the production of this chemical. As shown in the results of the complex marginal technology approach (Table 6), this could have important consequences for the accuracy of the final results when the Solvay route is included in the scenarios, particularly for ferric chloride (42 % $w/w$) where results vary by some 2.5-fold. For this chemical, the production of chlorine gas has an overall improved GHG emissions outcome when sodium hydroxide displaces sodium carbonate produced through the Solvay route, and this

**Table 6** cCF results (GWP) in kilograms CO$_2$-eq per megagram of sodium hypochlorite (13 % $w/w$) and ferric chloride (42 % $w/w$) produced using the complex marginal technology via CSIRO PEM and sodium hydroxide substituting sodium carbonate produced via Trona ore and Solvay process

| Scenario[a] | Substitution via | Sodium hypochlorite (13 % $w/w$) | Ferric chloride (42 % $w/w$) |
|---|---|---|---|
| 1 | Trona | 266 | 584 |
|   | Solvay | 314 | 214 |
| 2 | Trona | 281 | 621 |
|   | Solvay | 328 | 251 |
| 3 | Trona | 283 | 628 |
|   | Solvay | 316 | 219 |
| 4 | Trona | 284 | 629 |
|   | Solvay | 332 | 259 |

[a] Please check Table 4 for the details of the complex marginal mix associated with each scenario

explains the observed differences in results for ferric chloride (42 % $w/w$) using both sodium carbonate production routes.

In the case of sodium hypochlorite (13 % $w/w$), the associated burden of both chlorine gas and sodium hydroxide were required to be included, with the latter being a more significant input to its production. When the Solvay process route is assumed, a smaller environmental benefit is obtained when sodium hydroxide substitutes a smaller amount of sodium carbonate produced through this route than when the Trona ore process route is modelled; this explains why the GWP of sodium hypochlorite (13 % w/w) production via the Solvay route is slightly higher than when using the Trona ore route in Table 6. In summary, substitution plays an important role in the comprehensiveness of cCF studies with multifunctional outputs, and the use of alternate production routes is encouraged.

For the water treatment chemicals included in this study, the inclusion of key drivers such as carbon and fuel prices, as well as substitution alternatives, is crucial. The incorporation of economic modelling gives us a greatly enhanced understanding of the potential scale of variability in the results when
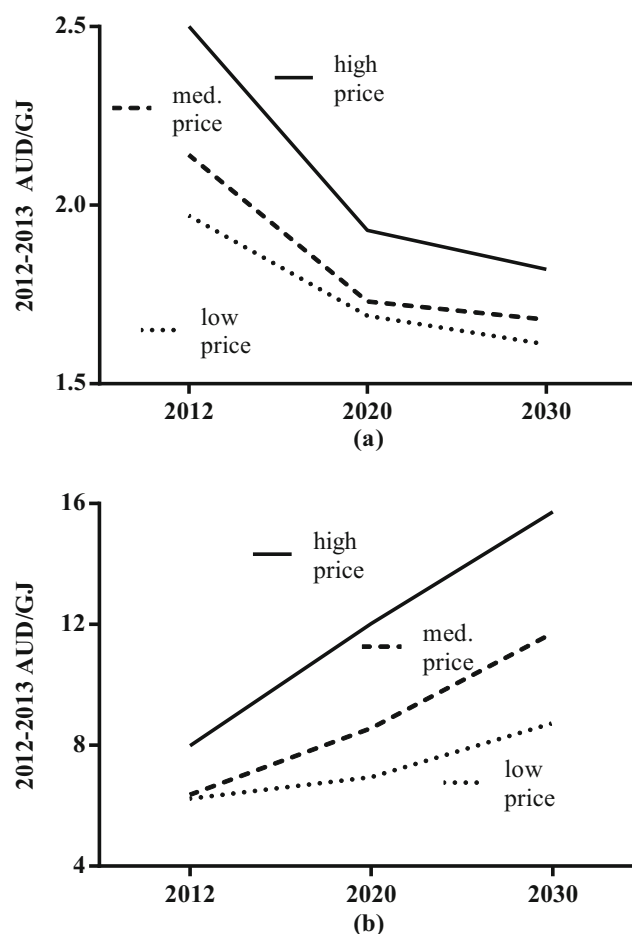


**Fig. 5** Low, medium and high price scenarios for **a** black coal and **b** natural gas affecting the marginal mix of technologies in 2030 in Australia (BREE 2012)

different scenarios are assessed. However, there are also limitations associated with the use of economic models, such as PEM, due to the uncertain nature of many of the parameters included. For example, the availability, performance and cost evolution of technologies is affected by innovation which could make any technology cheaper in the timeframe of analysis. Other shortcomings include full competitive markets and perfect foresight from market participants. In addition, the PEM used in this study does not include community acceptance which could have an impact in the uptake of technologies (William et al. 2012).

The implications of our results are significant for a wide range of stakeholders. In the case of LCA practitioners, scenarios need to be incorporated into cCFs in order to present the potential continuum of results arising from methodological assumptions that may have unknown but important consequences for the final outcomes. For example, the incorporation of scenarios in the modelling of ferric chloride (42 % w/w) production provides for a much more robust assessment of the likely environmental performance of this chemical in terms of the range of potential future results. At the same time, the production of sodium hypochlorite (13 % w/w) was shown to be relatively less likely to be adversely impacted by either the future electricity supply or the sodium carbonate production route chosen; this inconsistency in results between these two chemicals serves to further highlight the need for scenarios in cCFs to encapsulate the full spectrum of probable environmental repercussions. Aside from providing improved clarity on aspects of future chemicals supply, these insights present an opportunity for the water sector to expand the discussion surrounding future electricity supply, presently the single major contributor to the environmental impacts of potable water service provision (Lundie et al. 2004). The identification of the marginal supply mix of electricity for chlor-alkali chemicals production in Australia also contributes towards filling a knowledge gap recently identified in consequential analysis of potable water treatment and distribution in Australia (Lane et al. 2012).

## 4 Conclusions

Proper identification of future marginal technologies requires the inclusion of scenarios in order to manage the uncertainty associated with indirect effects. This exploratory cCF study for water treatment chemicals has demonstrated that, when electricity plays a significant role in the environmental impacts of a product or service, the common practice of using only one simple marginal technology in consequential studies is not recommended. We suggest the use of the complex marginal technology approach for long-term changes of the electricity market in consequential studies. When using a PEM, the incorporation of scenarios helps to understand the

nature of potential variability in the results. These are required to be relevant to the technology in question, such as the prices of carbon and fuel which are critical to electricity technologies in the long term.

Finally, the impacts of substitution should be considered carefully for different systems. While the inclusion of the Solvay route for sodium hydroxide substitution in the ferric chloride (42 % w/w) production system showed a reduced impact in terms of the GWP of this chemical, the same could not be said for sodium hypochlorite (13 % w/w). While substitution is the only way to solve multifunctionality in CLCIs, the use of only one substitution route is not recommended, unless it represents the only path possible. The incorporation of different production routes of the function to be substituted provides a clearer picture of the likely impacts associated with incorporating market information into cCF.

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